Predictive theory for light-ion reactions

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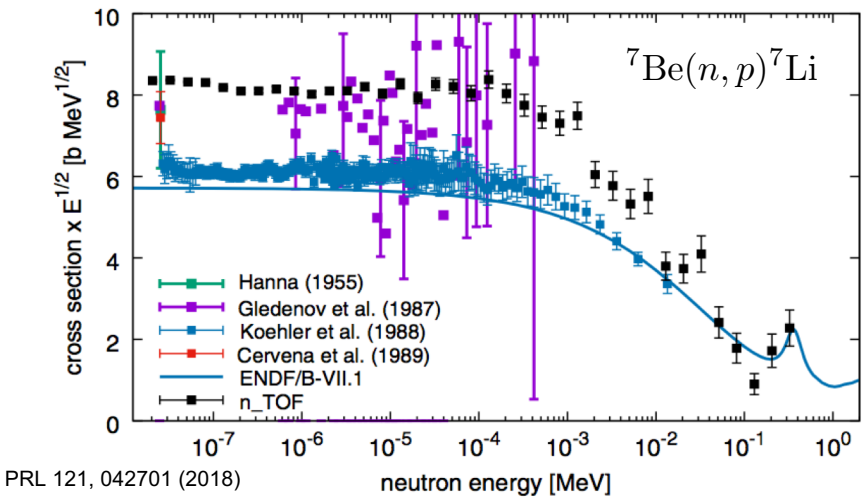
Background

- **We want to provide accurate nuclear data for:**
  - Big-bang and solar reaction rates that are difficult to measure
  - Fusion diagnostics
  - Improving accuracy of neutron cross section standards
- **Nuclear data here includes: nuclear energy levels, cross sections, angular distributions, polarization observables.**
- **Goal: Predict low-energy nuclear reactions by solving the quantum-mechanical equations for colliding nuclei made from interacting nucleons.**
- **Challenge: Simulating a nuclear many-body system is computationally expensive, makes it difficult to do uncertainty quantification of calculations.**



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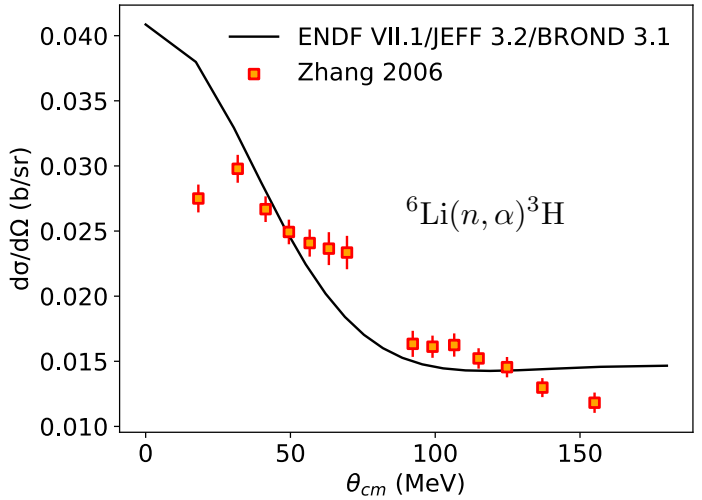
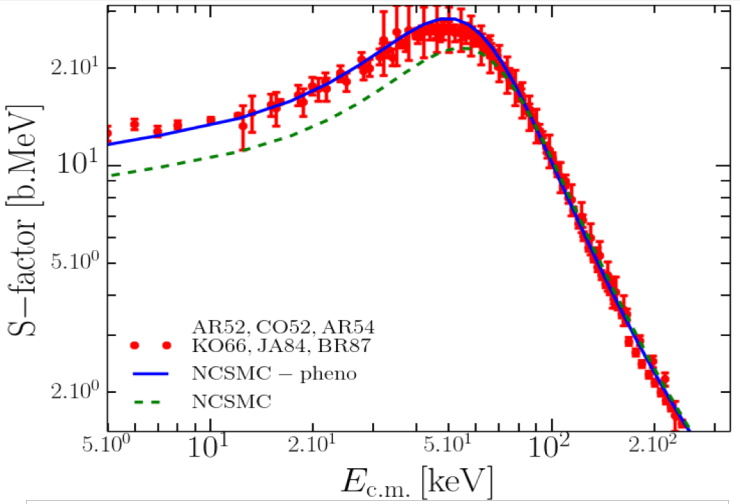
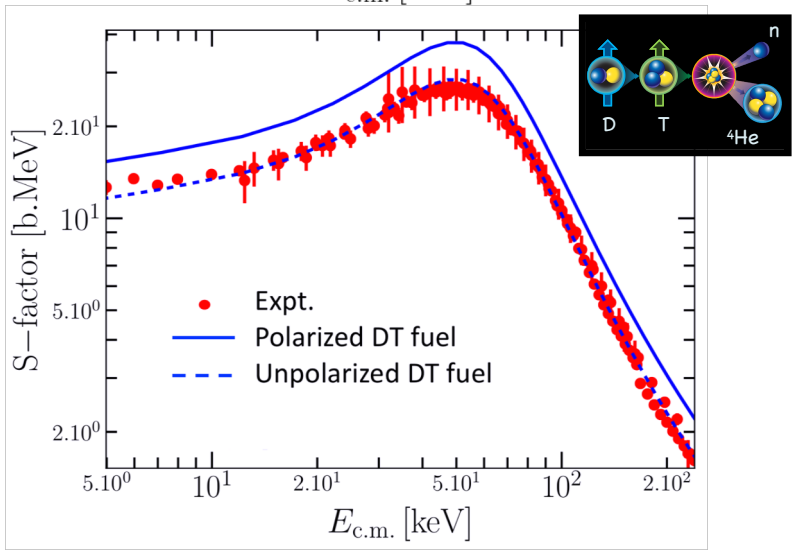


Computational Needs

Sole input is the interaction between the nucleons.

Typical runs take up significant part of the machine and require multiple runs.

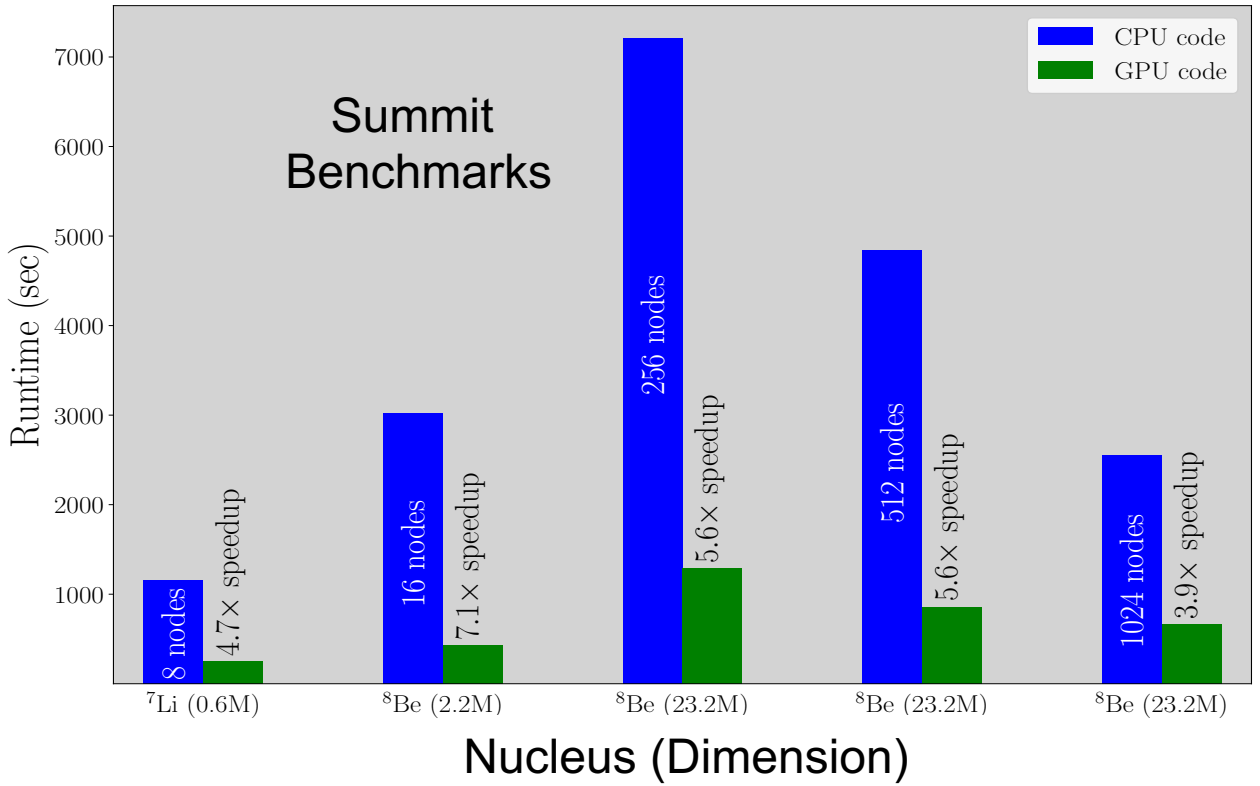




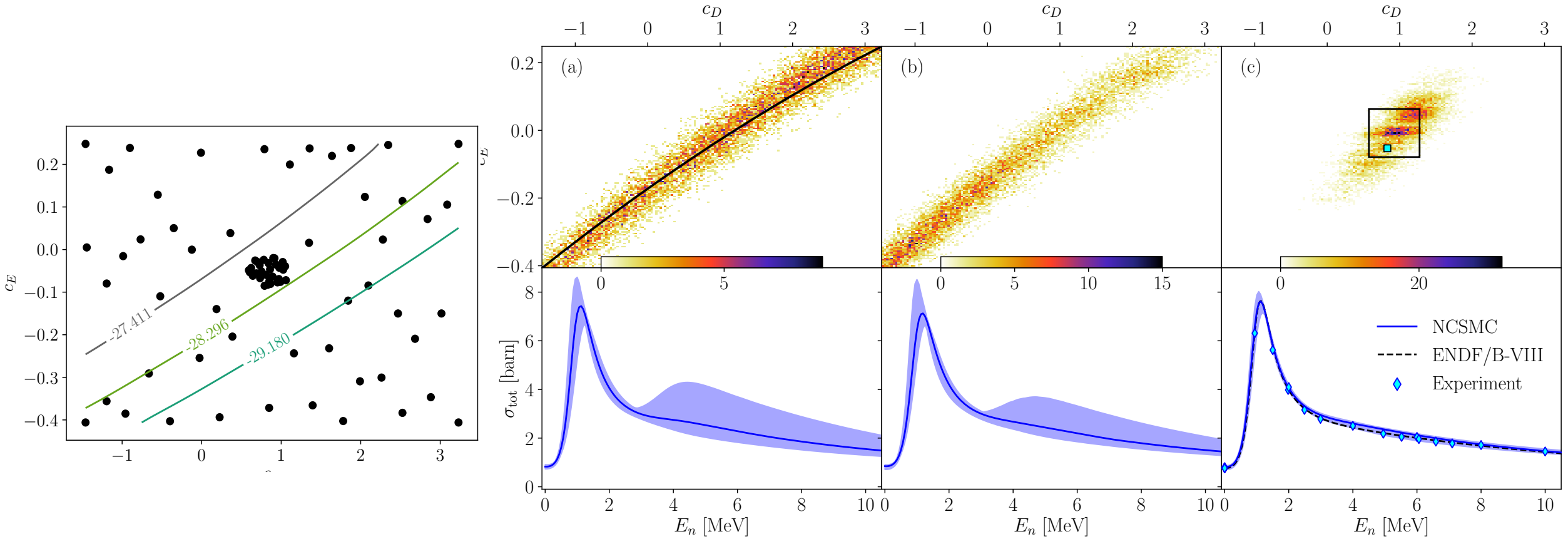
Current Hybrid(CPU+GPU) architectures

- Moving from traditional CPU-only architecture to GPUs has already resulted in significant speedups.
- Core computation algorithms required re-thinking to reduce memory footprint to minimize CPU-GPU transfers.
- However, at this stage the limited memory of GPU cards hinder moving to heavier systems.

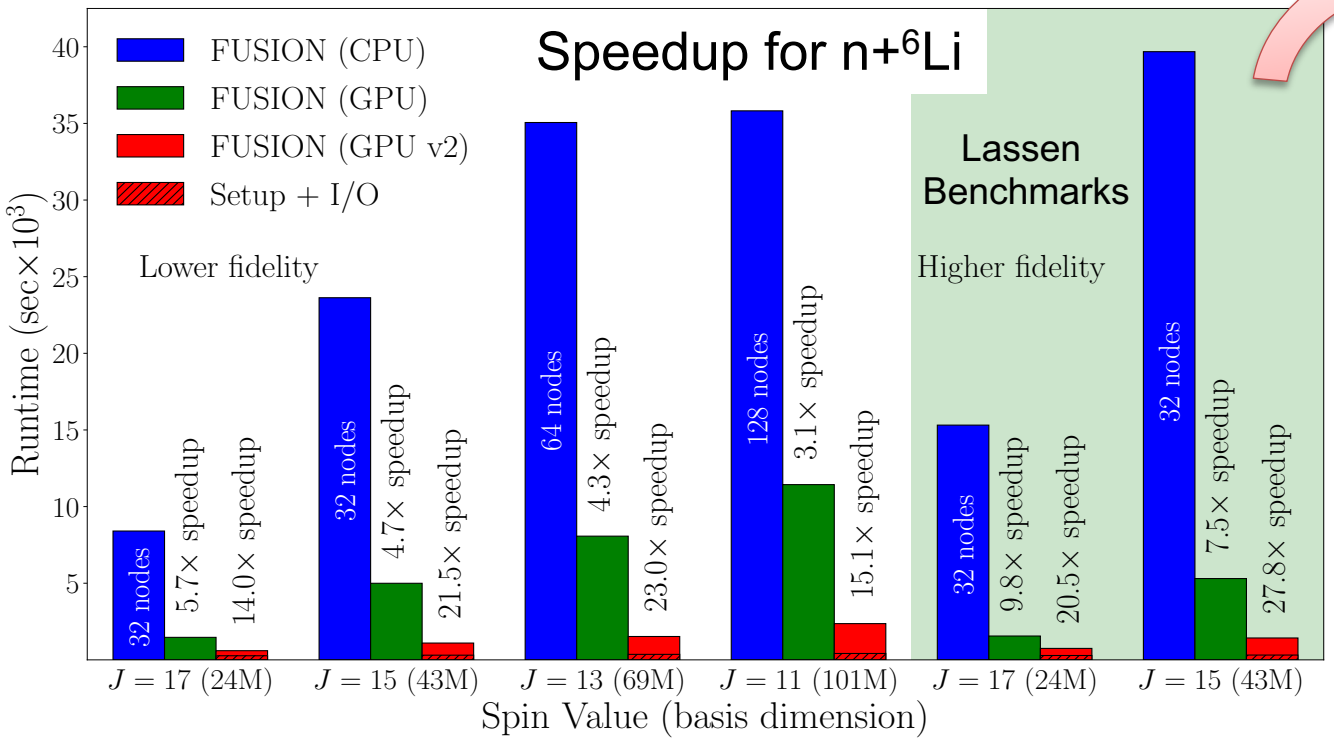
Speedup in calculation of nuclear states.

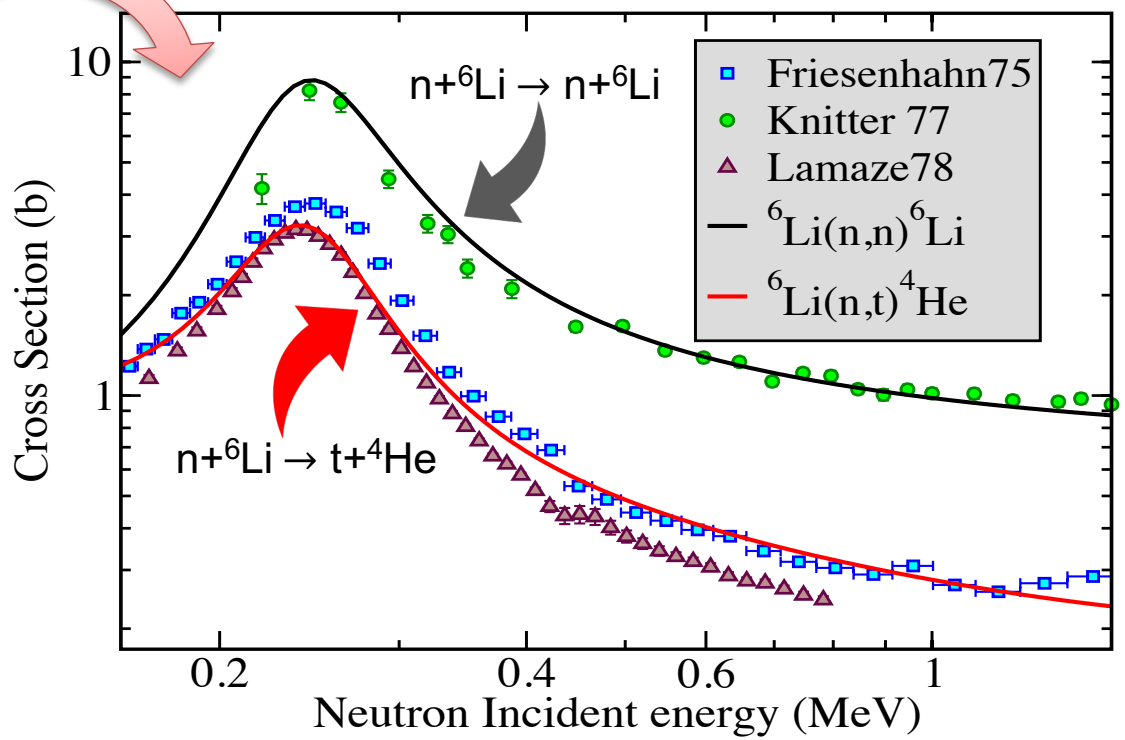


Accelerated codes coupled with Gaussian Process emulators allow for uncertainty quantification



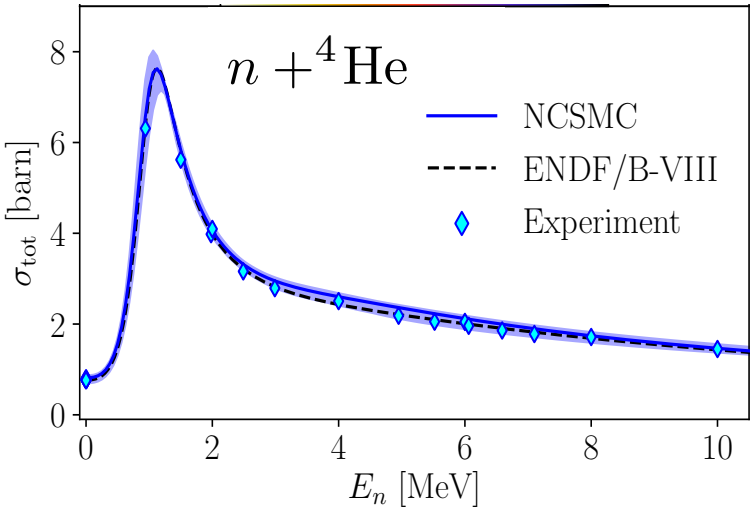
GPU-acceleration enables ab initio evaluation of n+^{6}Li reactions

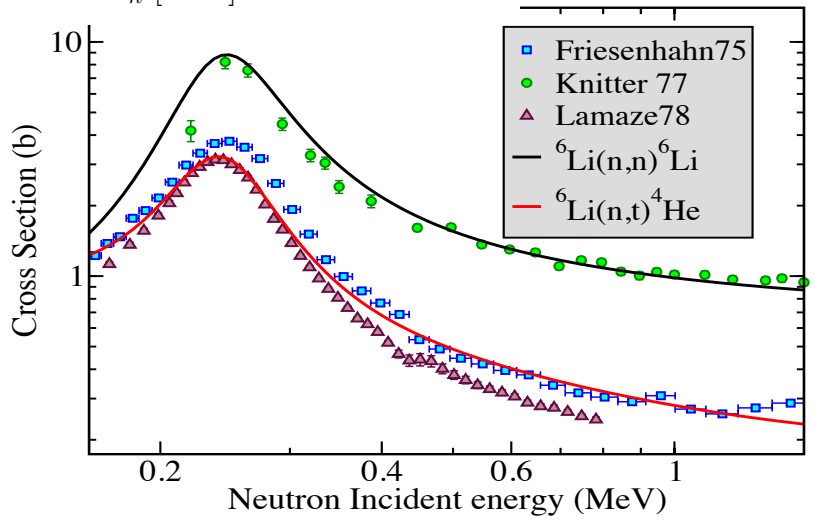




Outlook & Prospects

- Microscopic theories are now at the point where predictions of nuclear properties relevant to nuclear applications can be performed
- Additional effort required to push into heavier systems
- Mixed fidelity emulators to do UQ for expensive calculations?





Thank you!